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The Cambridge Structural Database: a quarter of a million crystal structures and rising
FH Allen - Acta Crystallographica Section B Structural Science, 2002 - dx.doi.org
... Chemical **connection table** (see text and Fig. ... Formal two-dimensional chemical **structure diagram** in terms of atom and bond ... Space group and **symmetry** operators. ...
Cited by 1140 - Web Search - journals.iucr.org - scripts.iucr.org - ncbi.nlm.nih.gov - all 6 versions »

SMILES. 2. Algorithm for generation of unique SMILES notation
D Weininger, A Weininger, JL Weininger - Journal of Chemical Information and Computer Sciences, 1989 - pubs.acs.org
... beyond 15. Partial characterization is therefore often attempted and is adequate for most **symmetry** perception problems. Such algorithms ...
Cited by 66 - Web Search - pubs.acs.org - csa.com

Computer storage and retrieval of generic chemical structures in patents, 2. GENSAL, a formal ...
JM Barnard, MF Lynch, SM Welford - Journal of Chemical Information and Computer Sciences, 1981 - pubs.acs.org
... FORMAL DESCRIPTION OF GENSAL **Structure Diagram** Input ... a routine to convert its output into the **connection table** ... that there are no **symmetry** considerations involved ...
Cited by 8 - Web Search

Chemical structure representation for information exchange Thomas Engel, Johann Gasteiger The ...
T Engel - Online Information Review, 2002 - emeraldinsight.com
... limitations of a **connection table** description: a ... Helson, HE (1999), "**Structure diagram** generation", Reviews ... numbering and constitutional **symmetry**", Journal of ...
Cited by 1 - Web Search - emeraldinsight.com - ingentaconnect.com - ingentaconnect.com

Chemical Abstracts Service Chemical Registry System. 13. Enhanced handling of stereochemistry
JE Blackwood, PEB Jr., SW Layten, DH Lillie, AH ... - Journal of Chemical Information and Computer Sciences, 1991 - pubs.acs.org
... search or display of stereochemistry in the **structure diagram**. ... the octa- hedral center in the **connection table** would be ... one or more of its **symmetry** axes leads ...
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Structural Search Codes for On-Line Compound Registration
LA Evans, MF Lynch, P Willett - Journal of Chemical Information and Computer Sciences, 1978 - pubs.acs.org
... rep- resentation, any unambiguous representation for a structure, eg, a **connection table** derived from an arbitrarily numbered **structure diagram**, may be used to ...
Web Search

Simulation and Evaluation of Chemical Synthesis. Representation and Manipulation of S tereochemis ...
WT Wipke, TM Dyottlb - J. Amer. Chem. Soc, 1974 - pubs.acs.org
... trans- form a three-dimensional structure or a two-dimensional structural diagram having wedged and hashed bonds into the ordered-list **connection table**, and to ...
Web Search

Computer Storage and Retrieval of Generic Chemical Structures in Patents, 16. The Refined Search: An ...
JD Holliday, MF Lynch - Journal of Chemical Information and Computer Sciences, 1995 - pubs.acs.org
... in which case they can be represented by a **structure diagram** or they ... are the full computer representation (the extended **connection table** representation3 or ECTR ...
Cited by 3 - Web Search

CML tools and information flow in atomic scale simulations
J Wakelin, P Murray-Rust, S Tyrrell, Y Zhang, HS ... - Mol. Simul, 2005 - eminerals.esc.cam.ac.uk
... of molecular mass, chemical **structure diagram** generation, topologi ... 5. Apply **symmetry** operations to generate the mini ... 6. Generate a **connection table** (CT) for the ...
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Chemical Markup, XML, and the Worldwide Web. 1. Basic Principles
P Murray-Rust, HS Rzepa - Journal of Chemical Information and Computer Sciences, 1999 - www-encore.enscm.fr
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CCL February 12, 1997 [004]

PREV UP NEXT

From:	badertscher &at& org.chem.ethz.ch (Martin Badertscher)
Date:	Wed, 12 Feb 1997 17:30:55 +0100
Subject:	perception algorithms for aromaticity etc.

Dimitris K. Agrafiotis wrote:

> We are trying to find some good algorithms for perceiving aromaticity,
> tautomerism and stereochemistry (RS, cis/trans) from a connection
> table, and algorithms for canonicalizing molecular graphs.

1. Canonicalizing molecular graphs
A molecular graph, or "constitution", can be coded as a connection table i more than one way. To prove that two connection tables code the same constitution is called the isomorphism problem. To solve the problem is notoriously expensive. One possible solution is to assign a canonical nam (or canonical connection table) to the constitutions. If two such names are the same, the constitutions are too. This involves the perception of topological symmetry. Many algorithms have been proposed, e.g., the far Morgan algorithm:

H. L. Morgan, J. Chem. Doc., Vol. 5 (1965) p. 107

Most of them, including the Morgan algorithm, suffer from the fact that they are not rigorous. Shelley has published an "almost rigorous" algorithm:

C. A. Shelley et al., J. Chem. Inf. Comput. Sci., Vol. 17, No. 2 (1977) p. 1

Ray Carhart, the wizzard, has found a counterexample (by summoning lo

R. E. Carhart, J. Chem. Inf. Comput. Sci., Vol. 18, No. 2 (1978) p. 108

As a reaction Shelley placed a brute force algorithm on top of his former one. The resulting construct is rigorous:

C. A. Shelley et al., J. Chem. Inf. Comput. Sci., Vol. 19, No. 4 (1979) p. 2

Due to Carhart's punishment the authors were too careful in writing their text. So the scientific community missed the fact that the problem was solved for almost 10 years. Chemists normally don't read mathematical journals where such problems are addressed in much more cryptic ways.

I can dig out the FORTRAN77 code of the complete algorithm to canonic a connection table. It could certainly be translated easily into a more appropriate language. The copyright is with Morton E. Munk, Prof. of Chemistry at Arizona State University. He is surely willing to share the code with you. Contact me if you are interested.

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2. Perceiving stereochemistry
This is a much more complicated problem as it (sensibly) involves the stability of molecules, not only mathematics. To my knowledge there is or a single algorithm published and coded that generates all stable stereoisomers out of a canonical connection table. It has its origin in Munk's lab too:

M. Razinger et al., J. Chem. Inf. Comput. Sci., Vol. 33, No. 6 (1993) p. 81

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3. Perceiving aromaticity
Before the question of perceiving aromaticity can be addressed, it must b clear what the results are used for. You have to clearly define what aromaticity is. This can be done in a purely mathematical way. Benzene, furane, and thiophene might be considered aromatic in this way, butadier could be non-aromatic, cyclobutadiene and cyclooctatetraene anti-aroma If you consider chemical behaviour such as reactivity, benzene and thiophene could be considered aromatic. Furane, butadiene, and cyclooctatetraene are non-aromatic. Cyclobutadiene is anti-aromatic and therefore rather unstable.

Martin Badertscher, head of radiochemistry,
dpt. of organic chemistry, federal institute of technology, Zurich, Switzerla

E-Mail: badertscher[AT]org.chem.ethz.ch

Similar Messages
06/08/1993: undergrad computational chem
08/01/1996: Re: CCL:M:Heat of formation calculation using MOPAC.
02/28/1995: conformational isomers
03/31/1995: Summary: Ring perception algorithms

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Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	2010	connection adj table	USPAT; EPO	OR	OFF	2006/01/19 20:48
L2	2	symmetry same 1	USPAT; EPO	OR	OFF	2006/01/19 20:48
L3	65	symmetry and 1	USPAT; EPO	OR	OFF	2006/01/19 20:49
L4	1614	structure adj diagram	USPAT; EPO	OR	OFF	2006/01/19 20:49
L5	2	3 and 4	USPAT; EPO	OR	OFF	2006/01/19 20:49

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CCL October 06, 1997 [009]

PREV UP NEXT

From:	Joerg Weiser <joerg { *at * } still3.chem.columbia.edu>
Date:	Mon, 06 Oct 1997 16:31:29 -0400
Subject:	Summary: Recognition of compounds from a connection table

Some time ago, I posted the following question:

"Do you know of any references that deal with the recognition of compounds (e.g stored in a compound library) from their connection tables?"

I received two answers. Thanks a lot.

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Try Ash, J., Chubb, P., Ward, S., Welford, S., Willet, P., Communiaction, Storage and Retrieval of Chemical Information, Ellis Horwood Series Chemical Science, Ellis Horwood Limited, Chichester, 1985.

It is not new, and some important modern developments are missing, but is is still a good overview about the basic principles and technology.

Dr. Wolf-D. Ihlenfeldt
Computer Chemistry Center, University of Erlangen-Nuernberg
Naegelsbachstrasse 25, D-91052 Erlangen (Germany)
Tel (+49)-(0)9131-85-6579 Fax (+49)-(0)9131-85-6566

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ftp://ftp.cs.ualberta.ca/pub/TechReports/1996/TR96-20/
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Alexander A. Oliferenko, Department of Organic Chemistry
Moscow State University, Lenin Hills, Moscow 119899, Russia

e-mail: alex ((at)) qsar.chem.msu.su; alex-qsar ((at)) technologist.c
Phone: 7 095 939 35 57

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Joerg Weiser phone: +1 212 8545143
Department of Chemistry +1 212 8548402
Columbia University
3000 Broadway MC 3140 fax: +1 212 6789039
New York, NY 10027 email: joerg "at@at" still3.chem.columbia.e
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02/24/1992: COMP Program for ACS MTG in San. Francisco
10/01/1998: Reminder - Fifth International Conference on Chemical Stru
01/05/1994: Summary of 1994 conferences list
01/18/1995: COMP Program for the Anaheim ACS Meeting
02/12/1997: perception algorithms for aromaticity etc.
03/06/1995: EHMO and ASED on organometallics (summary)

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